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FILE 'HCAPLUS' ENTERED AT 17:05:09 ON 13 JUL 2004

E PAGENKOPF B/AU

L1 33 E4

E YU M/AU

E YU MING/AU

L2 453 E3-52

L3 10 L1 AND L2

L4 1 L3 AND PYRROLES/TI

FILE 'REGISTRY' ENTERED AT 17:12:27 ON 13 JUL 2004

FILE 'HCAPLUS' ENTERED AT 17:12:29 ON 13 JUL 2004

L5 TRA L4 1- RN : 55 TERMS

FILE 'REGISTRY' ENTERED AT 17:12:29 ON 13 JUL 2004

L6 55 SEA L5

L7 30 L6 AND (C3 OR NC4)/ES

=> b hcap

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FILE COVERS 1907 - 13 Jul 2004 VOL 141 ISS 3

FILE LAST UPDATED: 12 Jul 2004 (20040712/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'HCAPLUS' FILE

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L4 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2004 ACS on STN

AN 2003:960478 HCAPLUS

DN 140:111237

ED Entered STN: 10 Dec 2003

TI A Powerful New Strategy for Diversity-Oriented Synthesis of Pyrroles from Donor-Acceptor Cyclopropanes and Nitriles

AU Yu, Ming; Pagenkopf, Brian L.

CS Department of Chemistry and Biochemistry, The University of Texas at Austin, Austin, TX, 78712, USA

SO Organic Letters (2003), 5(26), 5099-5101

CODEN: ORLEF7; ISSN: 1523-7060

PB American Chemical Society
DT Journal
LA English
CC 27-13 (Heterocyclic Compounds (One Hetero Atom))
AB Lewis acid-activated donor-acceptor cyclopropanes react with aliphatic, aromatic, and .alpha.,.beta.-unsatd. nitriles in a novel cascade [3 + 2] dipolar cycloaddn., dehydration, and tautomerization sequence to afford pyrroles in moderate to excellent overall yield. This cost-effective and regiospecific method is ideally suited for the preparation of combinatorial libraries.
ST pyrrole deriv prepn donor acceptor cyclopropane reaction nitrile; Lewis acid catalyst
IT Cycloaddition reaction
 ([3+2]; dipolar; diversity-oriented synthesis of pyrroles via Lewis acid-activated cycloaddn./dehydration/tautomerization reactions of various donor-acceptor cyclopropanes and nitriles)
IT Nitriles, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (aliphatic; diversity-oriented synthesis of pyrroles via Lewis acid-activated cycloaddn./dehydration/tautomerization reactions of various donor-acceptor cyclopropanes and nitriles)
IT Nitriles, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (aromatic; diversity-oriented synthesis of pyrroles via Lewis acid-activated cycloaddn./dehydration/tautomerization reactions of various donor-acceptor cyclopropanes and nitriles)
IT Cycloaddition reaction catalysts
 (dipolar; diversity-oriented synthesis of pyrroles via Lewis acid-activated cycloaddn./dehydration/tautomerization reactions of various donor-acceptor cyclopropanes and nitriles)
IT Dehydration reaction
 Tautomerization
 (diversity-oriented synthesis of pyrroles via Lewis acid-activated cycloaddn./dehydration/tautomerization reactions of various donor-acceptor cyclopropanes and nitriles)
IT Lewis acids
 RL: CAT (Catalyst use); USES (Uses)
 (diversity-oriented synthesis of pyrroles via Lewis acid-activated cycloaddn./dehydration/tautomerization reactions of various donor-acceptor cyclopropanes and nitriles)
IT Nitriles, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (.alpha.,.beta.-unsatd.; diversity-oriented synthesis of pyrroles via Lewis acid-activated cycloaddn./dehydration/tautomerization reactions of various donor-acceptor cyclopropanes and nitriles)
IT 27607-77-8, Trimethylsilyl trifluoromethane sulfonate
 RL: CAT (Catalyst use); USES (Uses)
 (diversity-oriented synthesis of pyrroles via Lewis acid-activated cycloaddn./dehydration/tautomerization reactions of various donor-acceptor cyclopropanes and nitriles)
IT 75-05-8, Acetonitrile, reactions 100-47-0, Benzonitrile, reactions 107-12-0, Propyl nitrile 628-20-6 630-18-2, Pivalonitrile 874-90-8, p-Methoxybenzonitrile 1885-38-7 6443-72-7 60838-50-8 72229-08-4 78932-45-3 78932-46-4 78932-48-6 90482-42-1 104623-05-4 361456-14-6 575444-76-7 635320-14-8 647836-52-0 647836-71-3 647836-72-4 647836-73-5
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (diversity-oriented synthesis of pyrroles via Lewis acid-activated cycloaddn./dehydration/tautomerization reactions of various donor-acceptor cyclopropanes and nitriles)

IT 936-12-9P 2199-52-2P 22186-92-1P 24363-49-3P 27172-04-9P
27188-97-2P 38597-58-9P 647836-43-9P 647836-44-0P 647836-46-2P
647836-48-4P 647836-57-5P 647836-58-6P 647836-59-7P 647836-60-0P
647836-61-1P 647836-62-2P 647836-63-3P 647836-64-4P 647836-65-5P
647836-66-6P 647836-67-7P 647836-68-8P 647836-69-9P 647836-70-2P
647836-74-6P 647836-75-7P 647836-76-8P 647836-77-9P 647836-78-0P
647836-79-1P 647836-80-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(diversity-oriented synthesis of pyrroles via Lewis acid-activated
cycloaddn./dehydration/tautomerization reactions of various
donor-acceptor cyclopropanes and nitriles)

RE.CNT 63 THERE ARE 63 CITED REFERENCES AVAILABLE FOR THIS RECORD

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DICTIONARY FILE UPDATES: 12 JUL 2004 HIGHEST RN 708973-81-3

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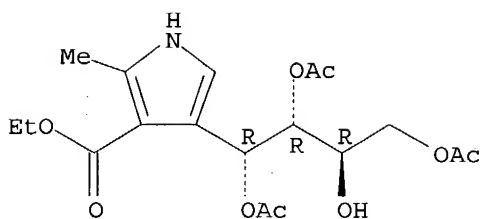
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L7 ANSWER 1 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 647836-79-1 REGISTRY
CN 1H-Pyrrole-3-carboxylic acid, 2-methyl-4-[(1R,2R,3R)-1,2,4-tris(acetyloxy)-
3-hydroxybutyl]-, ethyl ester (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C18 H25 N O9
SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)

Absolute stereochemistry.

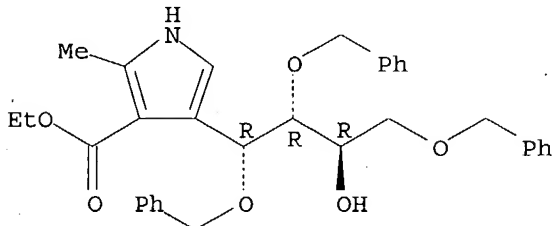


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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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RN 647836-78-0 REGISTRY
CN 1H-Pyrrole-3-carboxylic acid, 4-[(1R,2R,3R)-3-hydroxy-1,2,4-tris(phenylmethoxy)butyl]-2-methyl-, ethyl ester (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C33 H37 N O6
SR CA
LC STN Files: CA, CAPLUS
DT.CA Caplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)

Absolute stereochemistry.

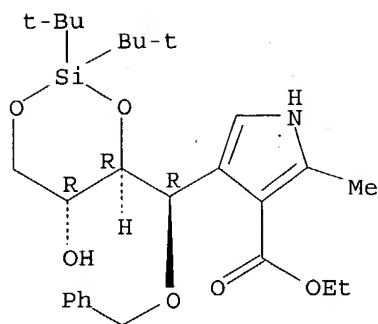


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L7 ANSWER 3 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 647836-77-9 REGISTRY
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FS STEREOSEARCH
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SR CA
LC STN Files: CA, CAPLUS
DT.CA Caplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)

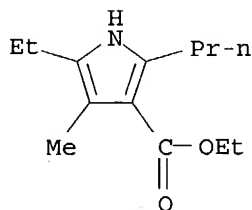
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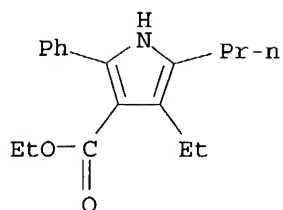
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RN 647836-69-9 REGISTRY
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(9CI) (CA INDEX NAME)
FS 3D CONCORD
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SR CA
LC STN Files: CA, CAPLUS
DT.CA Caplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)



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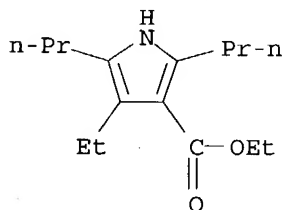
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(9CI) (CA INDEX NAME)
FS 3D CONCORD
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SR CA
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DT.CA Caplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)



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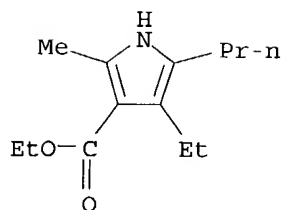
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DT.CA Caplus document type: Journal
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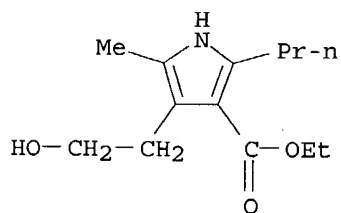
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(9CI) (CA INDEX NAME)
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RL.NP Roles from non-patents: PREP (Preparation)



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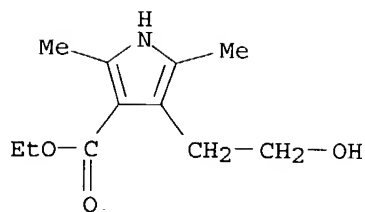
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RN 647836-65-5 REGISTRY
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FS 3D CONCORD
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SR CA
LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)



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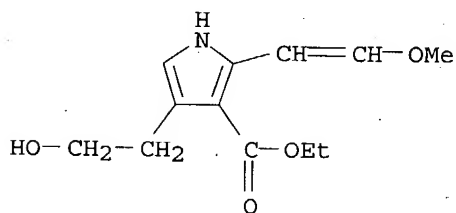
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LC STN Files: CA, CAPLUS
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)



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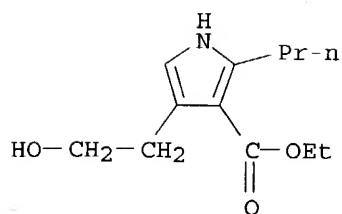
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SR CA
LC STN Files: CA, CAPLUS
DT.CA Caplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)



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1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L7 ANSWER 11 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 647836-62-2 REGISTRY
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FS 3D CONCORD
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SR CA
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RL.NP Roles from non-patents: PREP (Preparation)



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L7 ANSWER 12 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN

RN 647836-61-1 REGISTRY

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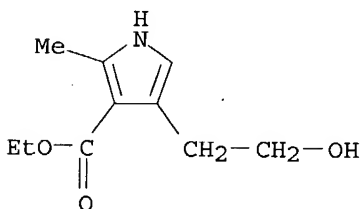
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SR CA

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RN 647836-60-0 REGISTRY

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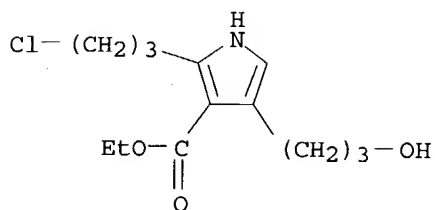
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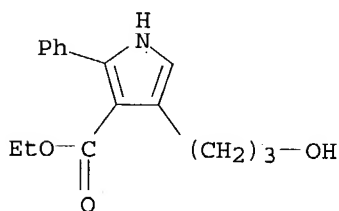


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L7 ANSWER 14 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 647836-59-7 REGISTRY
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(9CI) (CA INDEX NAME)
FS 3D CONCORD
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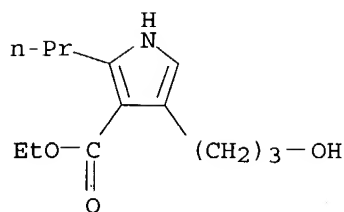


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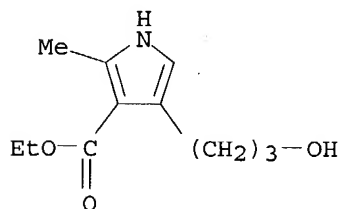
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RN 647836-58-6 REGISTRY
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(9CI) (CA INDEX NAME)
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DT.CA Caplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)



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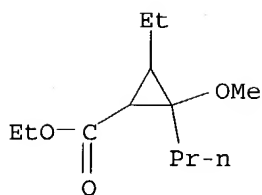
L7 ANSWER 16 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 647836-57-5 REGISTRY
CN 1H-Pyrrole-3-carboxylic acid, 4-(3-hydroxypropyl)-2-methyl-, ethyl ester
(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C11 H17 N O3
SR CA
LC STN Files: CA, CAPLUS
DT.CA Caplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

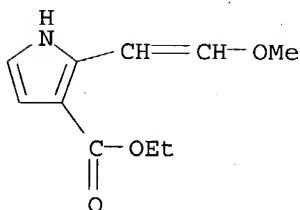
L7 ANSWER 17 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 647836-52-0 REGISTRY
CN Cyclopropanecarboxylic acid, 3-ethyl-2-methoxy-2-propyl-, ethyl ester
(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H22 O3
SR CA
LC STN Files: CA, CAPLUS
DT.CA Caplus document type: Journal
RL.NP Roles from non-patents: RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L7 ANSWER 18 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 647836-48-4 REGISTRY
CN 1H-Pyrrole-3-carboxylic acid, 2-(2-methoxyethenyl)-, ethyl ester (9CI)
(CA INDEX NAME)
FS 3D CONCORD
MF C10 H13 N O3
SR CA
LC STN Files: CA, CAPLUS
DT.CA Caplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)

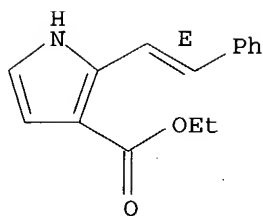


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L7 ANSWER 19 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 647836-46-2 REGISTRY
CN 1H-Pyrrole-3-carboxylic acid, 2-[(1E)-2-phenylethenyl]-, ethyl ester (9CI)
(CA INDEX NAME)
FS STEREOSEARCH
MF C15 H15 N O2
SR CA
LC STN Files: CA, CAPLUS
DT.CA Caplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation)

Double bond geometry as shown.

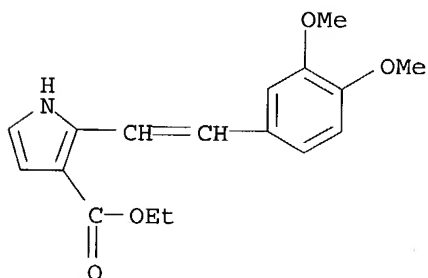


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L7 ANSWER 20 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 647836-44-0 REGISTRY
 CN 1H-Pyrrole-3-carboxylic acid, 2-[2-(3,4-dimethoxyphenyl)ethenyl]-, ethyl ester (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C17 H19 N O4
 SR CA
 LC STN Files: CA, CAPLUS
 DT.CA Caplus document type: Journal
 RL.NP Roles from non-patents: PREP (Preparation)

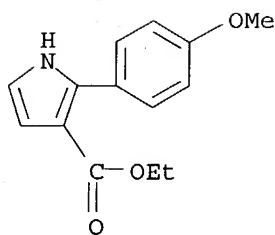


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

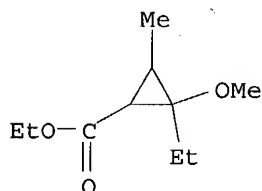
L7 ANSWER 21 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
 RN 647836-43-9 REGISTRY
 CN 1H-Pyrrole-3-carboxylic acid, 2-(4-methoxyphenyl)-, ethyl ester (9CI) (CA INDEX NAME)
 FS 3D CONCORD
 MF C14 H15 N O3
 SR CA
 LC STN Files: CA, CAPLUS
 DT.CA Caplus document type: Journal
 RL.NP Roles from non-patents: PREP (Preparation)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

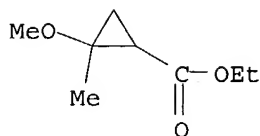
L7 ANSWER 22 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 635320-14-8 REGISTRY
CN Cyclopropanecarboxylic acid, 2-ethyl-2-methoxy-3-methyl-, ethyl ester
(9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C10 H18 O3
SR CA
LC STN Files: CA, CAPLUS, CASREACT
DT.CA Caplus document type: Journal
RL.NP Roles from non-patents: RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

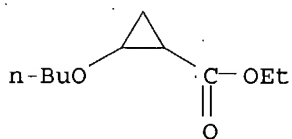
L7 ANSWER 23 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 78932-46-4 REGISTRY
CN Cyclopropanecarboxylic acid, 2-methoxy-2-methyl-, ethyl ester (9CI) (CA
INDEX NAME)
FS 3D CONCORD
MF C8 H14 O3
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, CHEMINFORMRX
(*File contains numerically searchable property data)
DT.CA Caplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

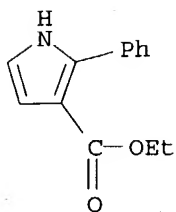
L7 ANSWER 24 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 78932-45-3 REGISTRY
CN Cyclopropanecarboxylic acid, 2-butoxy-, ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C10 H18 O3
LC STN Files: BEILSTEIN*, CA, CAPLUS, CHEMINFORMRX
(*File contains numerically searchable property data)
DT.CA Caplus document type: Journal
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent);
NORL (No role in record)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE)
6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L7 ANSWER 25 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 38597-58-9 REGISTRY
CN 1H-Pyrrole-3-carboxylic acid, 2-phenyl-, ethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C13 H13 N O2
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, TOXCENTER
(*File contains numerically searchable property data)
DT.CA Caplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation)
RL.NP Roles from non-patents: PREP (Preparation); RACT (Reactant or reagent)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L7 ANSWER 26 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN

RN 27188-97-2 REGISTRY

CN 1H-Pyrrole-3-carboxylic acid, 2-propyl-, ethyl ester (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Pyrrole-3-carboxylic acid, 2-propyl-, ethyl ester (8CI)

FS 3D CONCORD

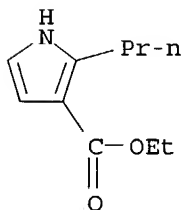
MF C10 H15 N O2

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

DT.CA Caplus document type: Journal

RL.NP Roles from non-patents: PREP (Preparation)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L7 ANSWER 27 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN

RN 27172-04-9 REGISTRY

CN 1H-Pyrrole-3-carboxylic acid, 5-methyl-2-propyl-, ethyl ester (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN Pyrrole-3-carboxylic acid, 5-methyl-2-propyl-, ethyl ester (8CI)

FS 3D CONCORD

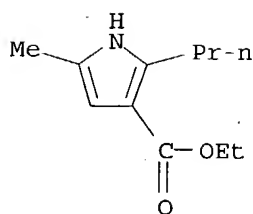
MF C11 H17 N O2

LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

DT.CA Caplus document type: Journal

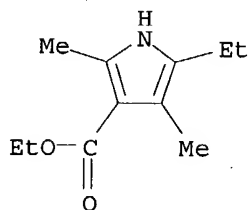
RL.NP Roles from non-patents: PREP (Preparation)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L7 ANSWER 28 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 22186-92-1 REGISTRY
CN 1H-Pyrrole-3-carboxylic acid, 5-ethyl-2,4-dimethyl-, ethyl ester (9CI)
(CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Pyrrole-3-carboxylic acid, 5-ethyl-2,4-dimethyl-, ethyl ester (8CI)
FS 3D CONCORD
MF C11 H17 N O2
CI COM
LC STN Files: BEILSTEIN*, CA, CAPLUS, CHEMCATS, TOXCENTER
(*File contains numerically searchable property data)
DT.CA Caplus document type: Journal; Patent
RL.P Roles from patents: PREP (Preparation)
RL.NP Roles from non-patents: PREP (Preparation); PRP (Properties)

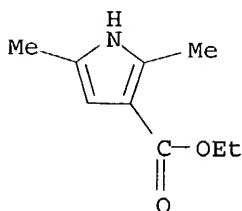


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

8 REFERENCES IN FILE CA (1907 TO DATE)
8 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L7 ANSWER 29 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 2199-52-2 REGISTRY
CN 1H-Pyrrole-3-carboxylic acid, 2,5-dimethyl-, ethyl ester (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Pyrrole-3-carboxylic acid, 2,5-dimethyl-, ethyl ester (6CI, 7CI, 8CI)
OTHER NAMES:
CN 2,5-Dimethylpyrrole-3-carboxylic acid ethyl ester
CN Ethyl 2,5-dimethylpyrrole-3-carboxylate
CN NSC 19437
FS 3D CONCORD

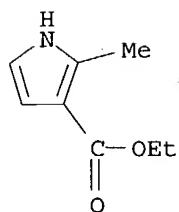
MF C9 H13 N O2
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CSCHEM,
HODOC*, IFICDB, IFIPAT, IFIUDB, SPECINFO, TOXCENTER
(*File contains numerically searchable property data)
DT.CA Caplus document type: Journal; Patent
RL.P Roles from patents: RACT (Reactant or reagent)
RL.NP Roles from non-patents: ANST (Analytical study); PREP (Preparation);
PRP (Properties); RACT (Reactant or reagent); NORL (No role in record)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

29 REFERENCES IN FILE CA (1907 TO DATE)
29 REFERENCES IN FILE CAPLUS (1907 TO DATE)
6 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L7 ANSWER 30 OF 30 REGISTRY COPYRIGHT 2004 ACS on STN
RN 936-12-9 REGISTRY
CN 1H-Pyrrole-3-carboxylic acid, 2-methyl-, ethyl ester (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Pyrrole-3-carboxylic acid, 2-methyl-, ethyl ester (6CI, 7CI, 8CI)
OTHER NAMES:
CN 3-(Ethoxycarbonyl)-2-methylpyrrole
CN 3-Ethoxycarbonyl-2-methyl-1H-pyrrole
CN Ethyl 2-methylpyrrole-3-carboxylate
CN NSC 81361
FS 3D CONCORD
MF C8 H11 N O2
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS,
CHEMINFORMRX, IFICDB, IFIPAT, IFIUDB, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)
DT.CA Caplus document type: Journal; Patent
RL.P Roles from patents: RACT (Reactant or reagent)
RL.NP Roles from non-patents: ANST (Analytical study); PREP (Preparation);
PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES
(Uses); NORL (No role in record)
RLD.NP Roles for non-specific derivatives from non-patents: FORM (Formation,
nonpreparative)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

45 REFERENCES IN FILE CA (1907 TO DATE)
 1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
 45 REFERENCES IN FILE CAPLUS (1907 TO DATE)
 13 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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